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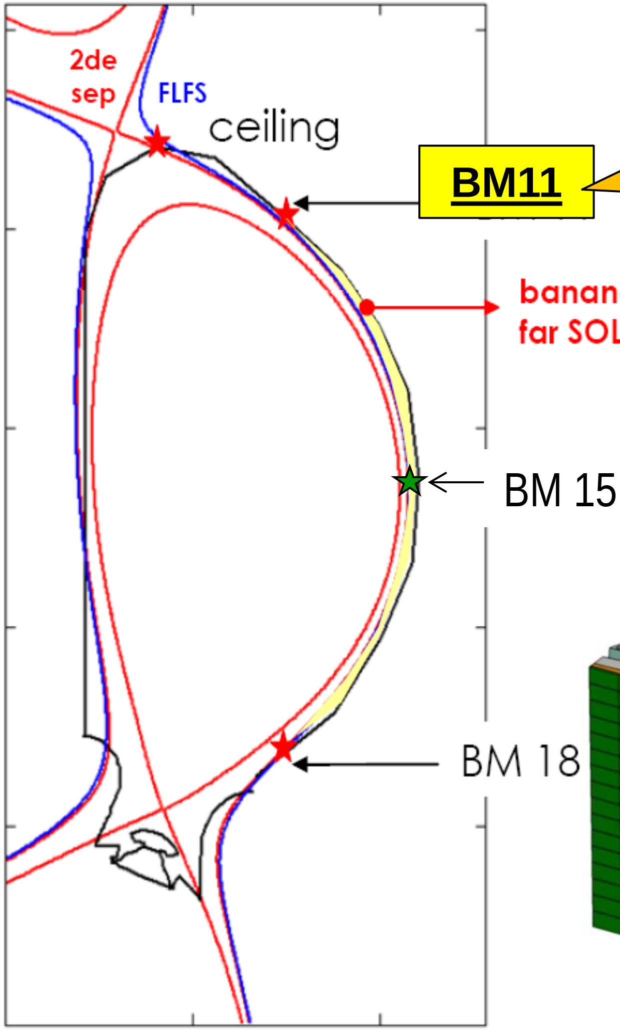
Atomic data for Be and W used in simulations by the ERO code

D.Borodin[a], S.Brezinsek[a], C.Björkas[b], D.Kondratyev[a], A.Kirschner[a], M.Stamp[c], E.Marenkov[f], A.Kreter[a], B.Unterberg[a], M.Laengner[a], D.Matveev[a], D.Reiser[a], Ch.Linsmeier[a] and the JET-EFDA contributors

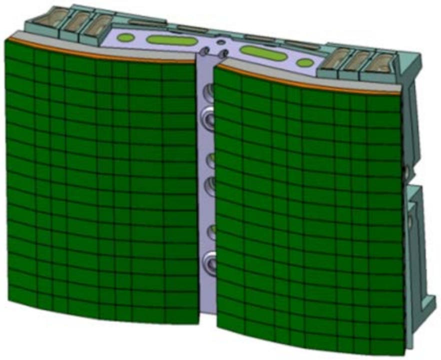
ET-EFDA, Culham Science Centre, Abingdon, OX14 3DB, UK
[a]Institute of Energy and Climate Research - Plasma Physics, Forschungszentrum Jülich GmbH, Association EURATOM-FZJ, Partner in the Trilateral Euregio Cluster, Jülich, Germany
[b]EURATOM-Tekes, Department of Physics, P.O. Box 43, FI-00014 University of Helsinki, Finland [c]EURATOM/CCFE Fusion Association, Culham Science Centre, Abingdon, OX14 3DB, UK
[f]National Research Nuclear University MEPhI, 31 Kashirskoe sh., 115409 Moscow, Russian Federation

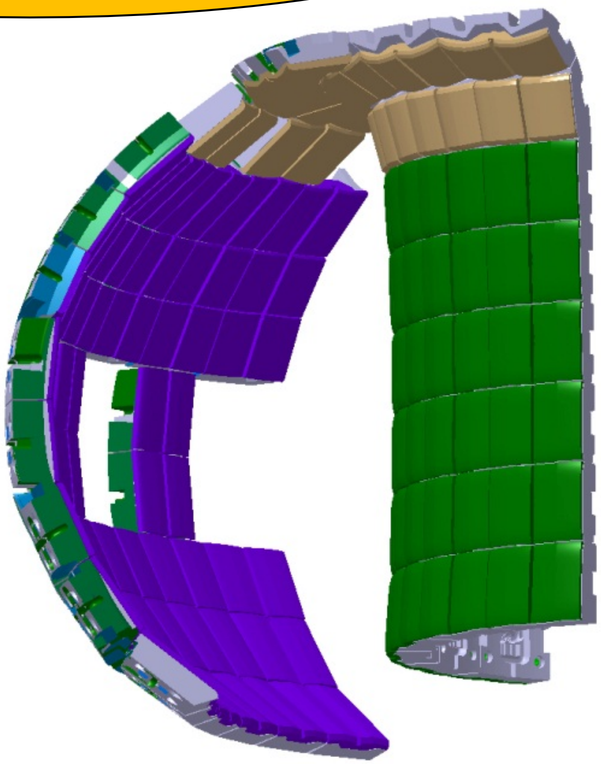
ITER Be wall – BM erosion



FLFS close to 2nd separatrix =>
First PFC ***life time*** estimates assuming
limiter-like contact on outboard BM11

<u>Be</u>
+ low Z
- high erosion

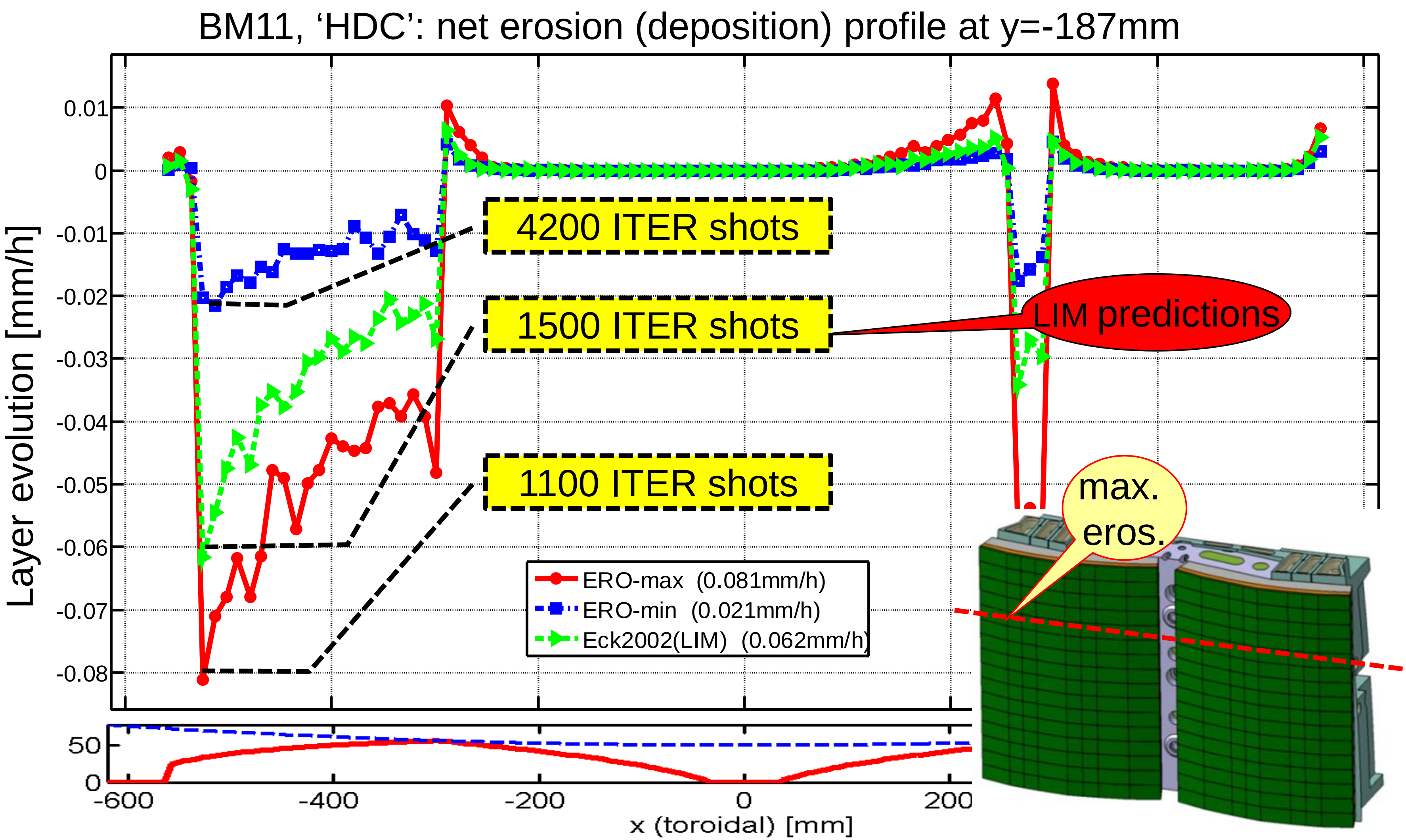




- *Blanket module (BM) shapes optimized for heat loads (P.C.Stangeby)*

<u>Aim</u> – predictive modelling of ITER, including first wall life time

Sputter yields assumptions and net erosion



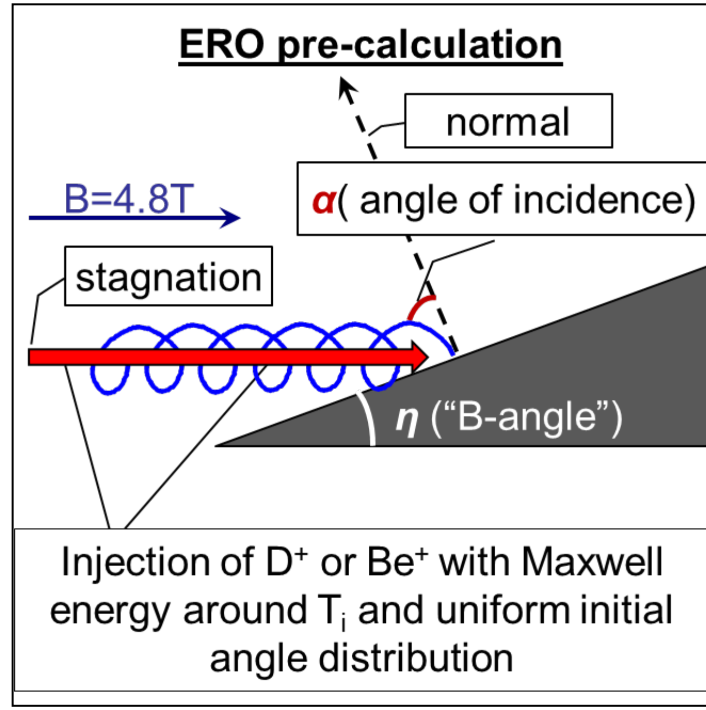
Sputtering data determined the outcome!

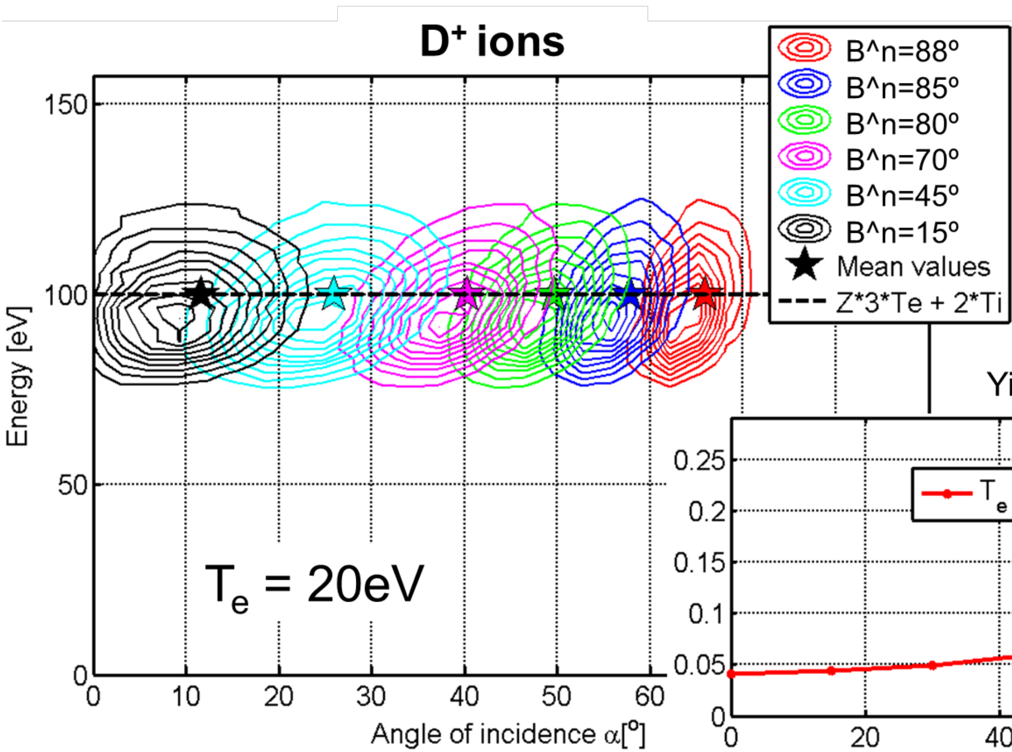
PFMC-2011

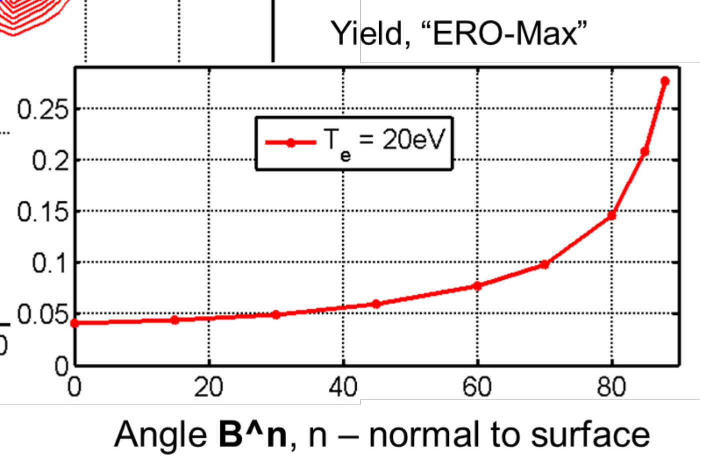
Sputtering by BG plasma (and intrinsic Be)

"integration" produces effective sputter yields:

$$Y(E_{in}, \alpha_{in}) = Y(E_{in}, 0) * A(E_{in}, \alpha_{in})$$

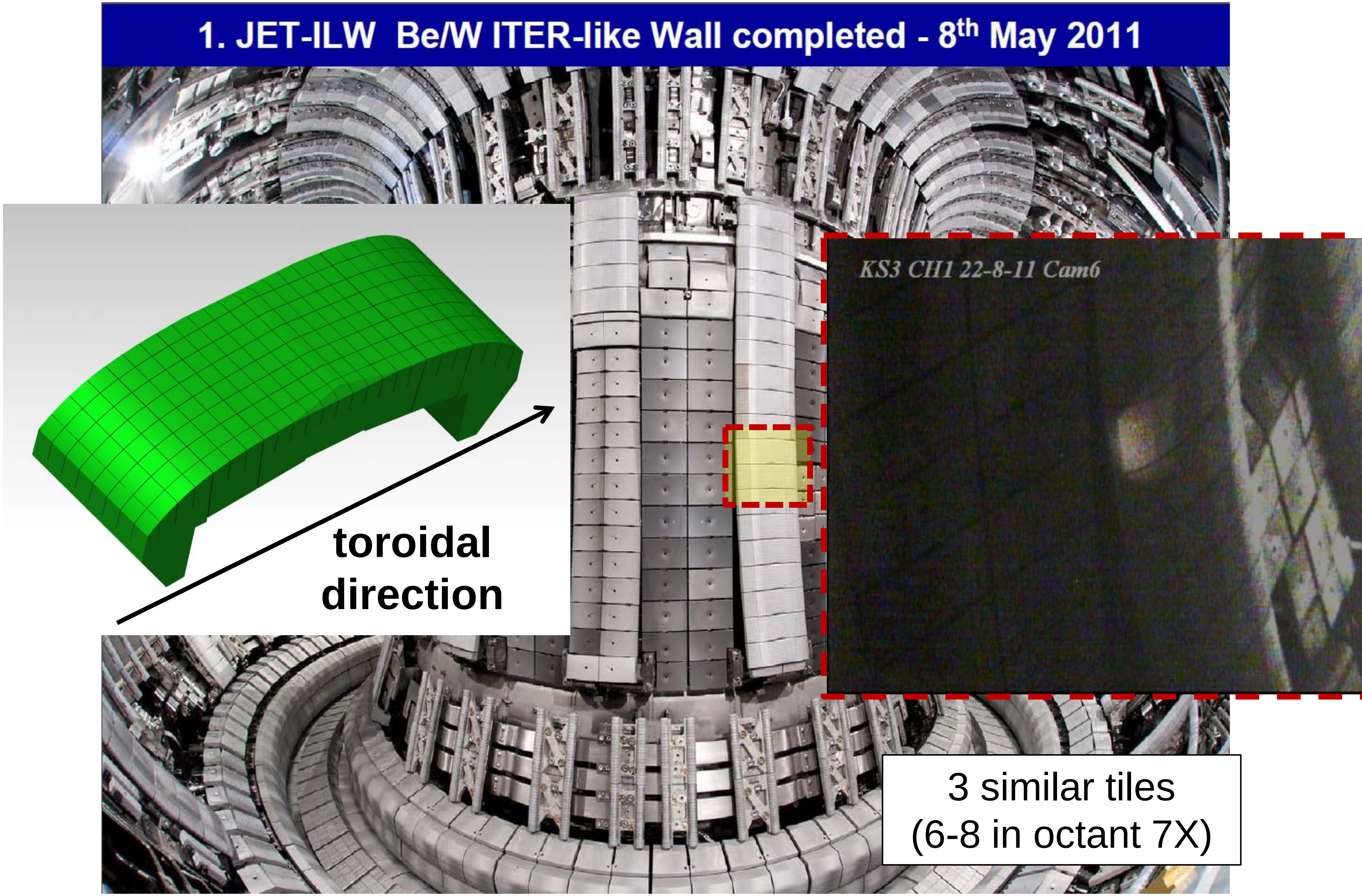






„ERO-min" – MD/BCA data for 50% D surface content

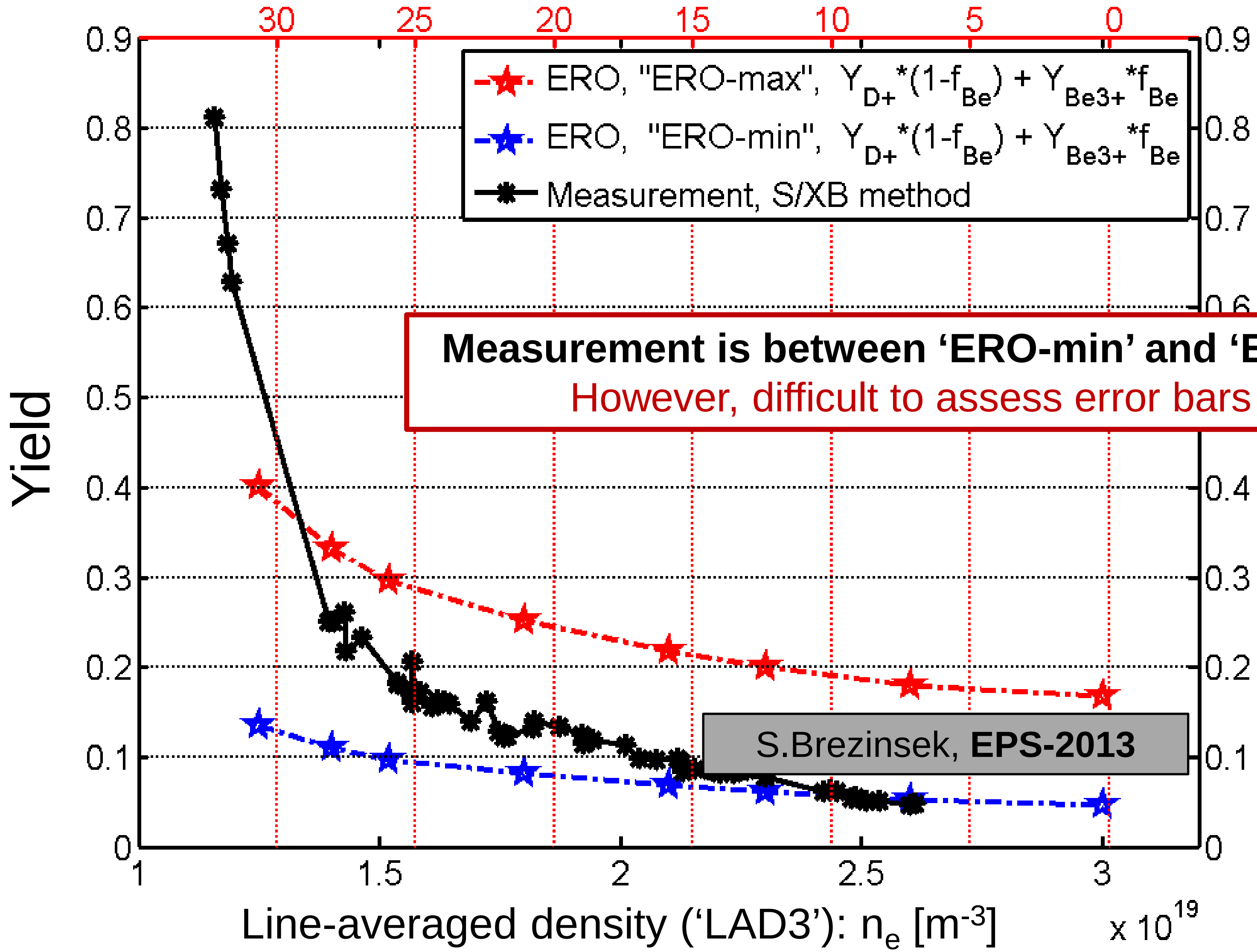
Solid Be Limiter of JET ILW



Yields: ERO and S/XB method, JET ILW

PFMC-2013

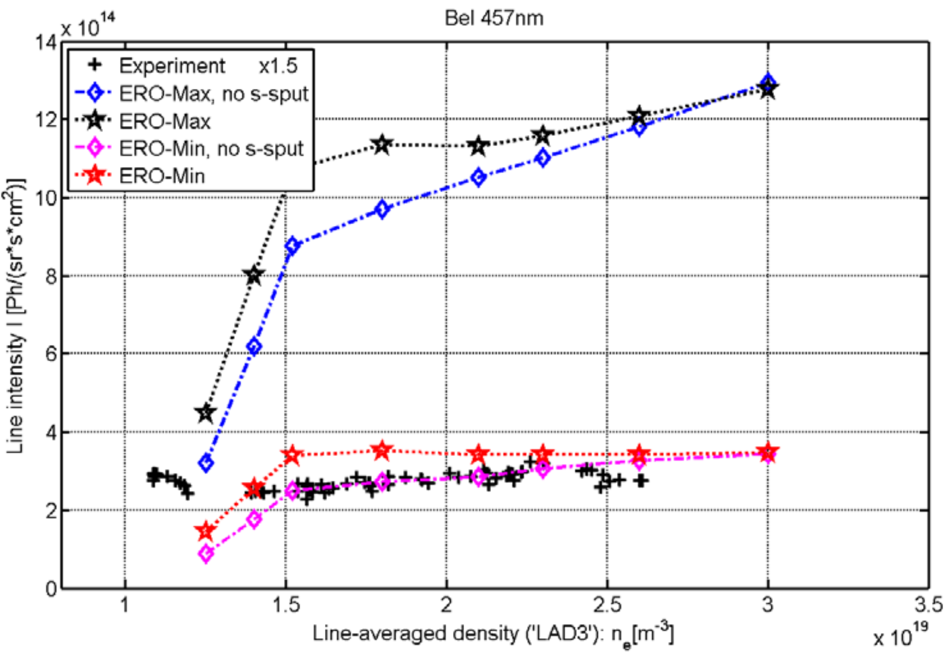
Effective empiric T_e[eV], from the BeII line ratios

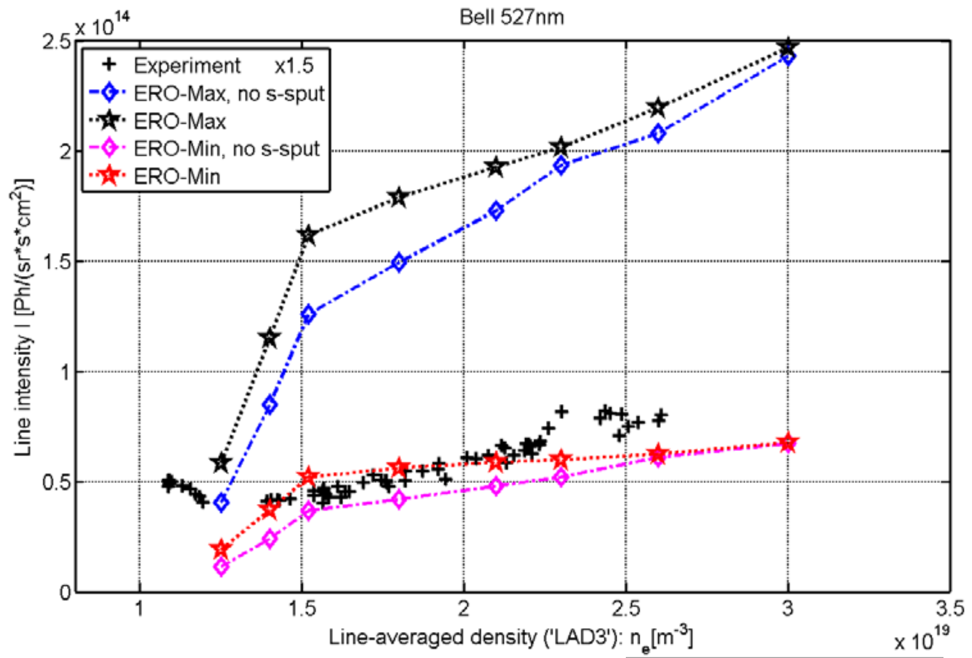


Measurement is between 'ERO-min' and 'ERO-max'!
However, difficult to assess error bars . . .

S.Brezinsek, **EPS-2013**

ERO&Experiment: BeII light





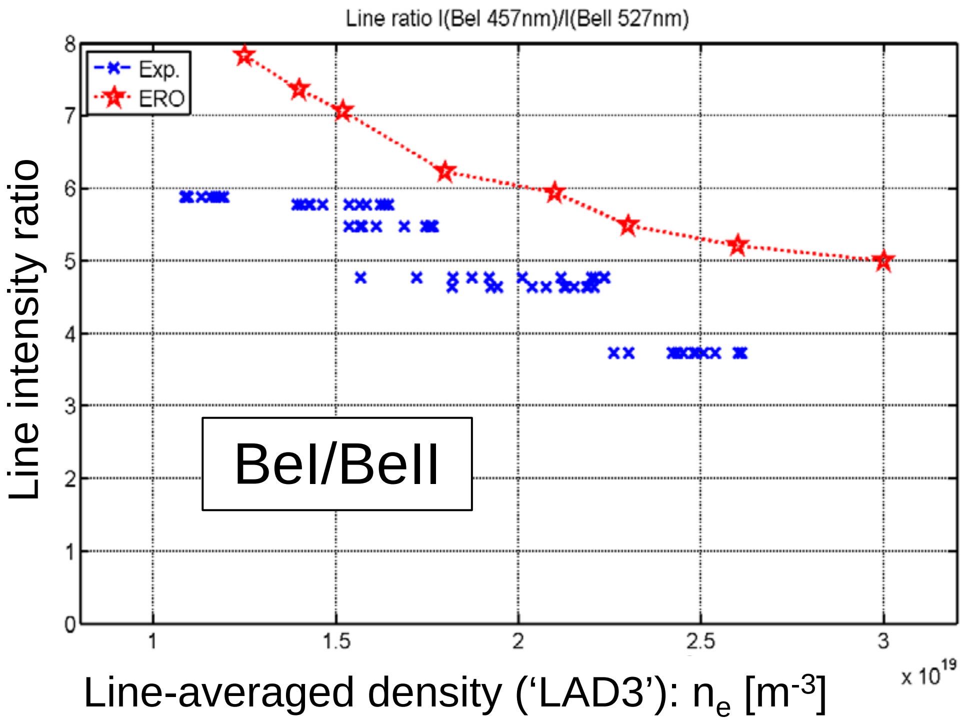
PFMC-2013

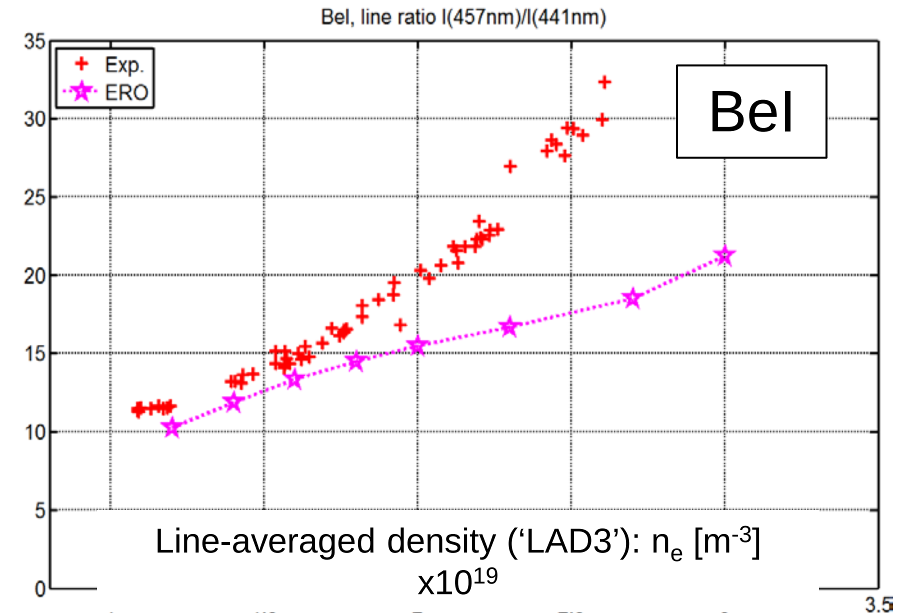
1) „ERO-Min“ still about factor 1.5 too large!
2) Effect of self-sputtering is reasonable but not as significant as schould be.
3) Growing trend reproduced

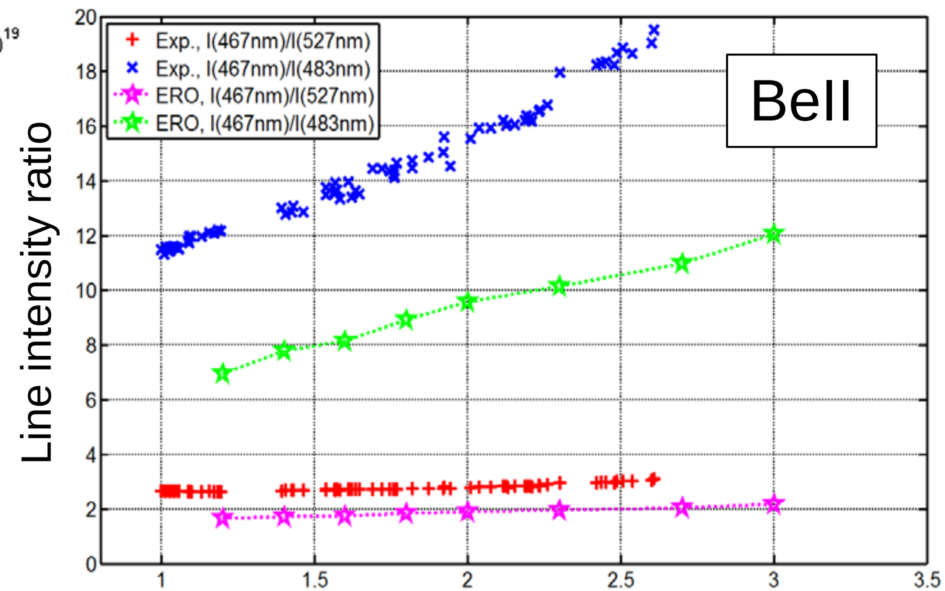
D-flux correction by Dγ
Icreases this by 50%!
So, factor 2-3!!!

Lower yields „ERO-min“ correspond to 50% D surface content . . .

ERO&Experiment: line ratios







Atomic data (ADAS '96'), 3D **plasma parameter** configuration and ERO simulated Be **transport** and plasma parameter lead to line ratio agreement within factor 2 or even better!

“ERO-BM” version (3D tile shaping)

ITER BM11 life time
D.Borodin, PFMC-2011

Previous 2D LIM simulations
S.Carpentier

JET ILW erosion
PSI-2012, PFMC-2013

W, Be, Be-D

Tore Supra (**DITS**)
S.Panayotis, EPS-2013

C, H-C

EAST (**MAPES**)
R.Ding, PFMC-2013

C (He and Ar plasma,),
*W, **Be proxy**?*

ERO Universal geometry
D.Matveev, ongoing

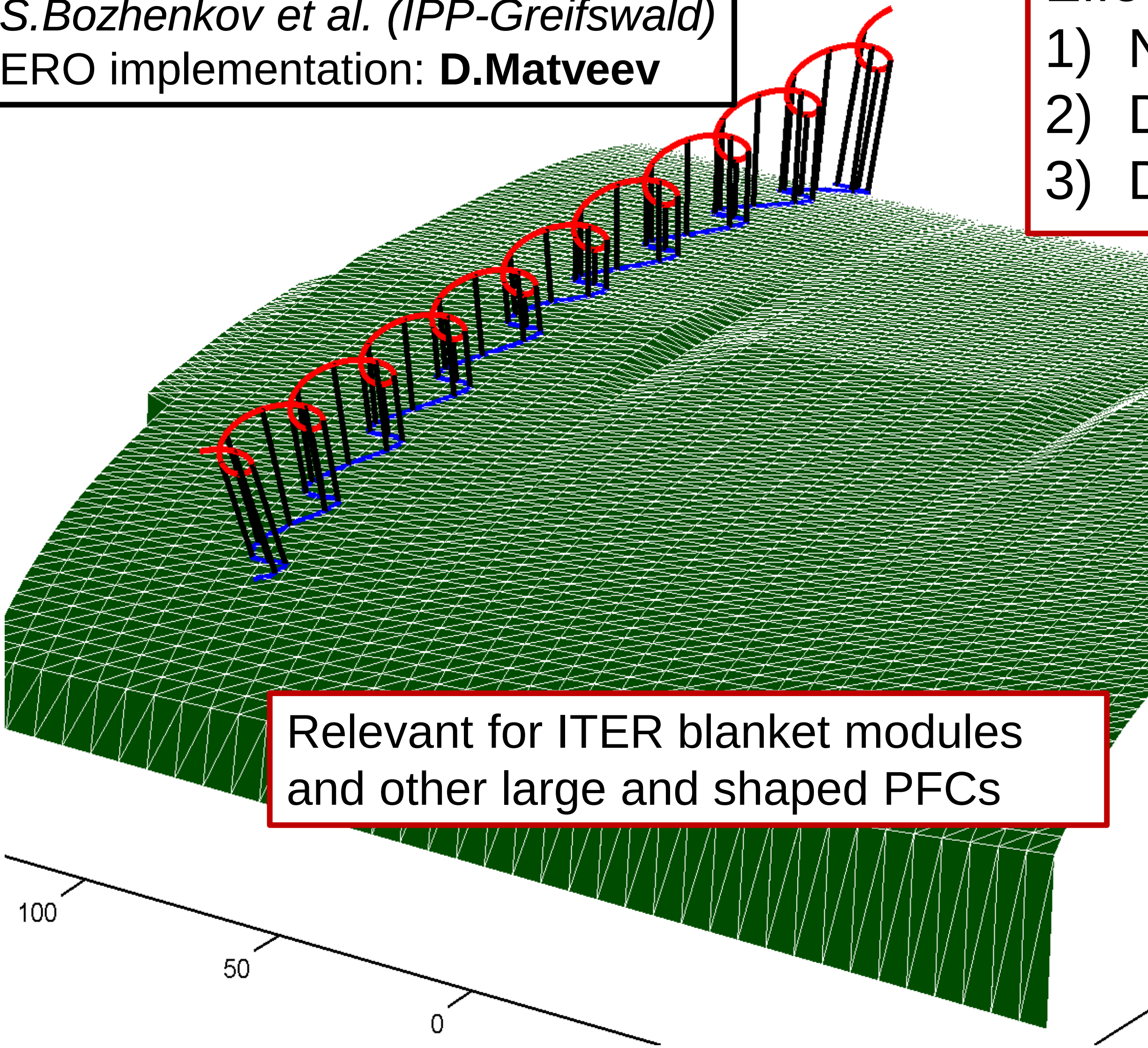
ERO-DIVIMP coupling
D.Elder (ITER contact)
Just started . . .

Benchmark with WALDYN
K.Schmid, **BM8?!..**
Just agreed . . .

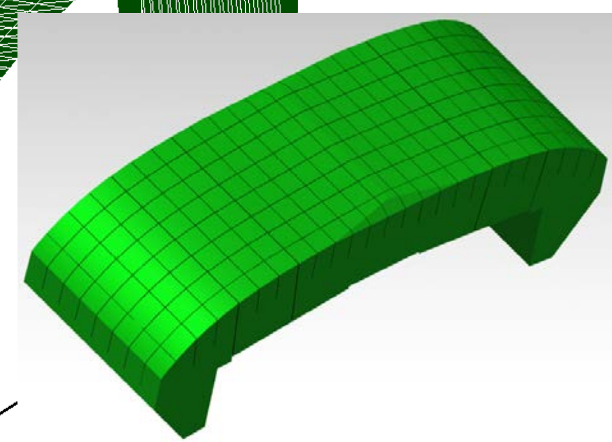
3D ERO-code: universal geometry

Based on 'MeshLib' library
S.Bozhenkov et al. (IPP-Greifswald)
ERO implementation: **D.Matveev**

Effective algorithms for:
1) Normal to surface
2) Distance to surface
3) Distance along field line



Relevant for ITER blanket modules and other large and shaped PFCs



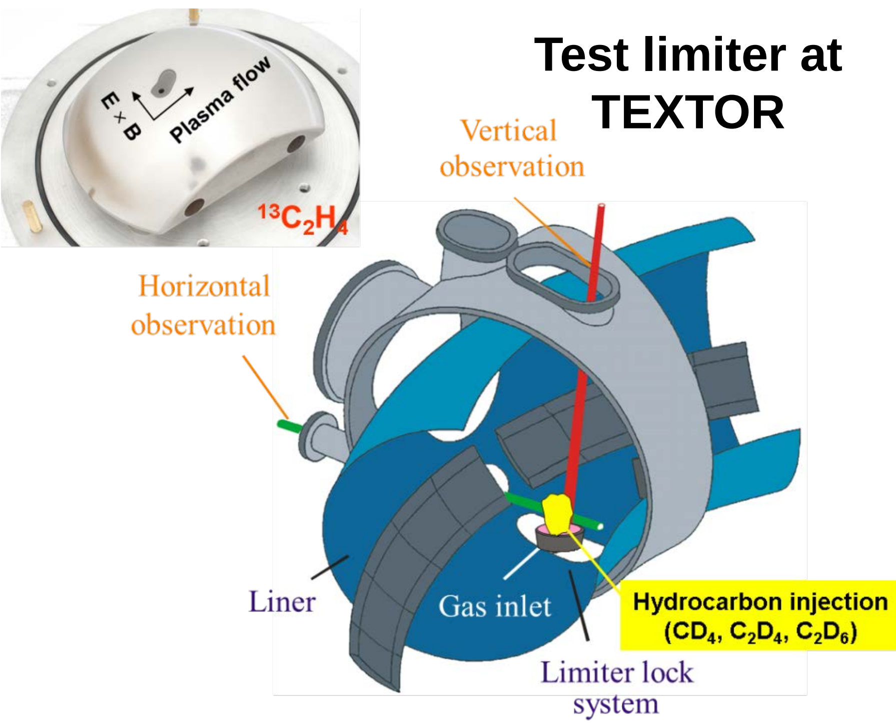
Motivation for ERO2.0

1) Over 20 years of development, worth general re-thinking
2) Many developers (physicists!)
3) Code performance issues
4) Code structure / readability issues
5) Well-established tool for ITER predictions
6) Well benchmarked against various experiments

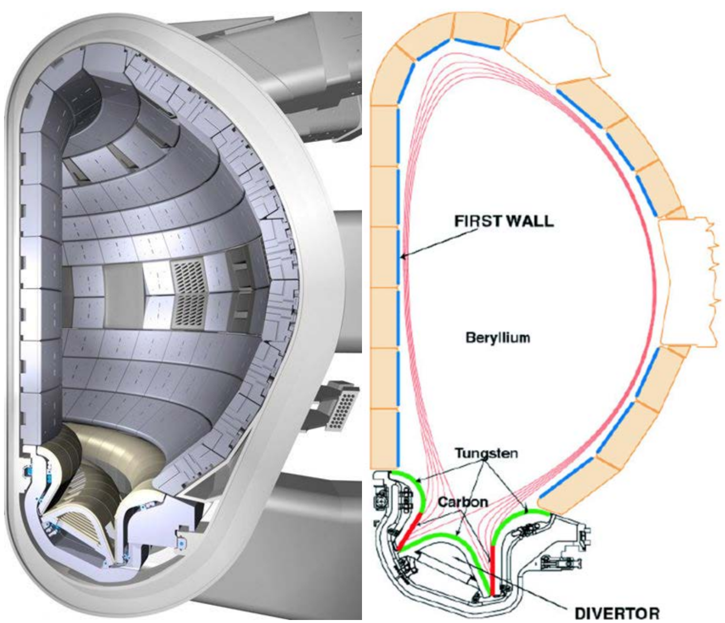
Massive parallelization

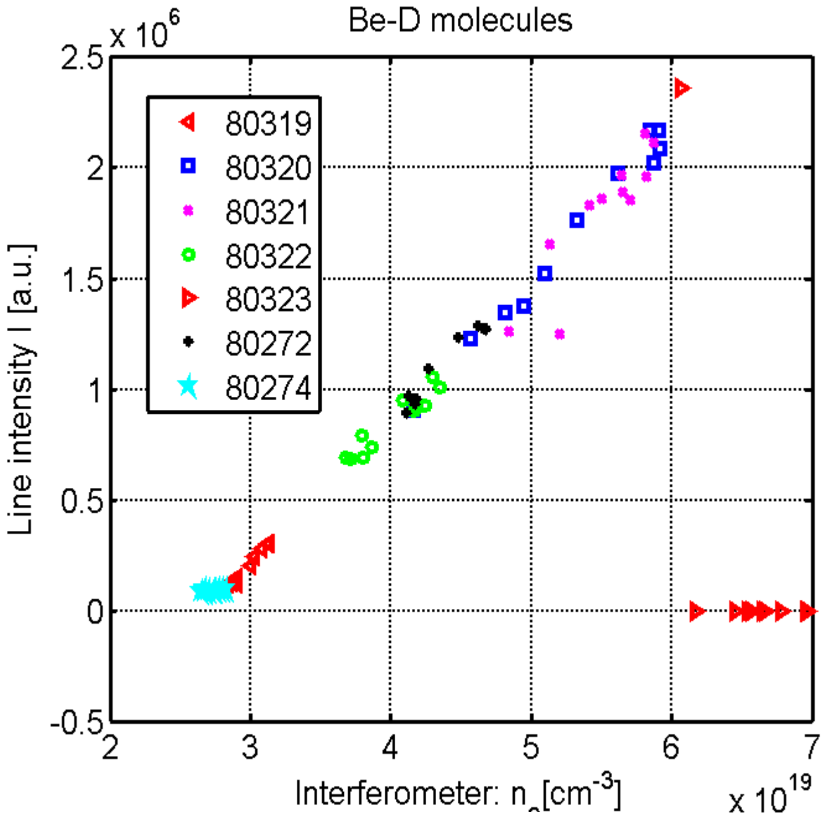
Aim: 'full-scale' device simulations w/o sacrifice of detail:

Test limiter at TEXTOR

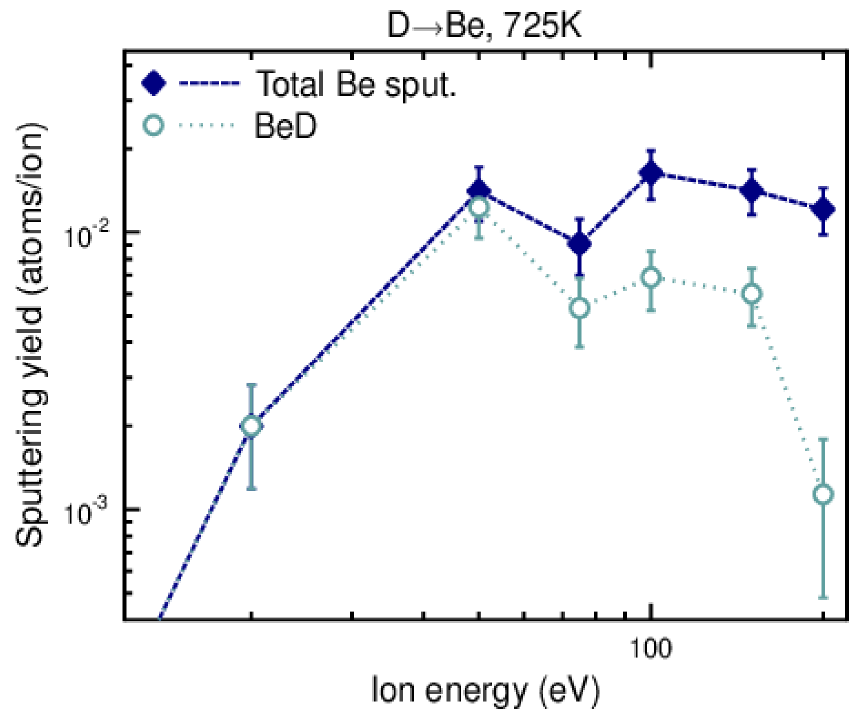


ITER





$n_e[m^{-2}]$

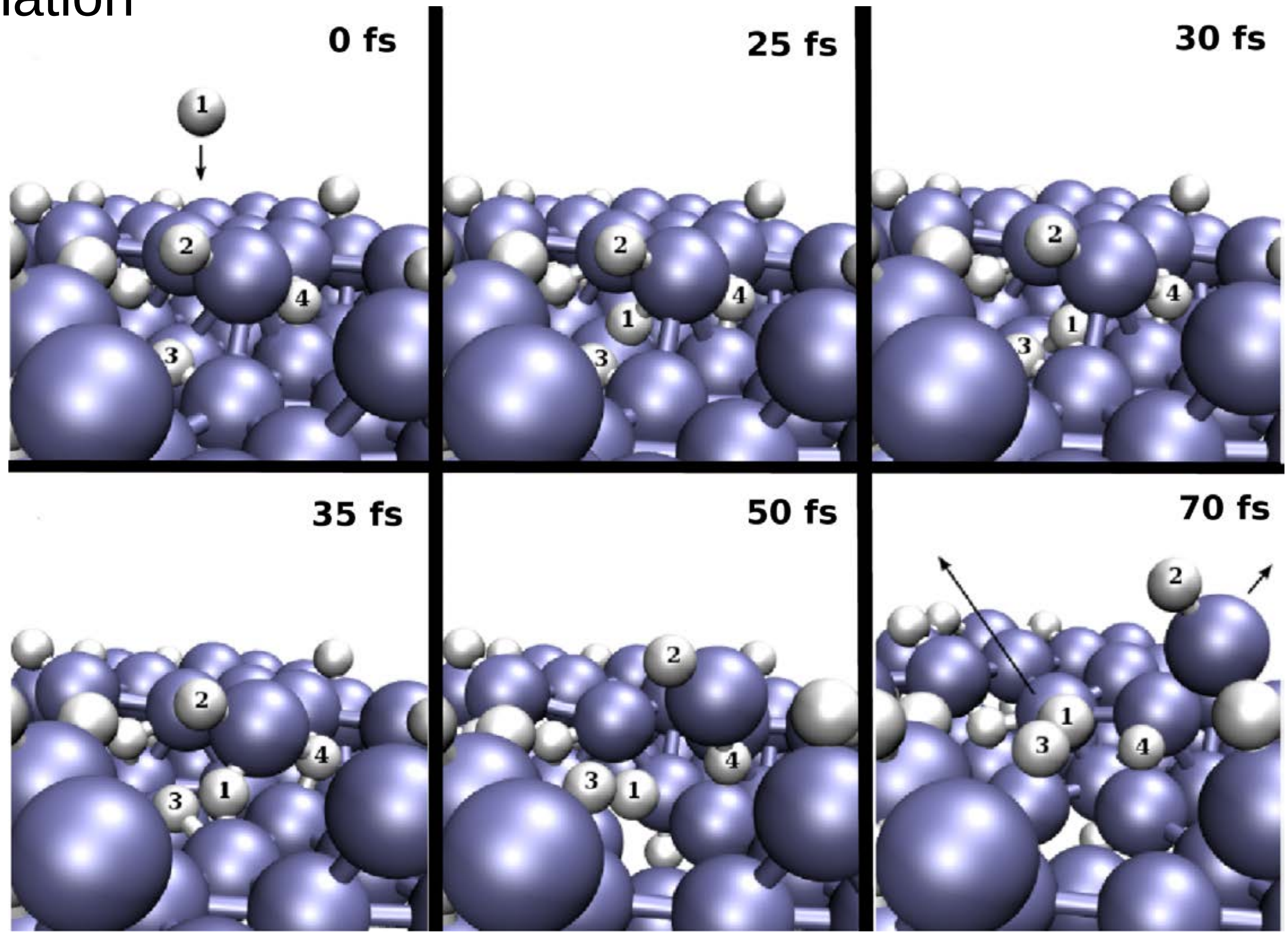


Be-D implementation in ERO – C.Bjoerkas et al, PSI-2012

May act as an important release mechanism, affecting other intesities ! . .
Further consideration is necessary.

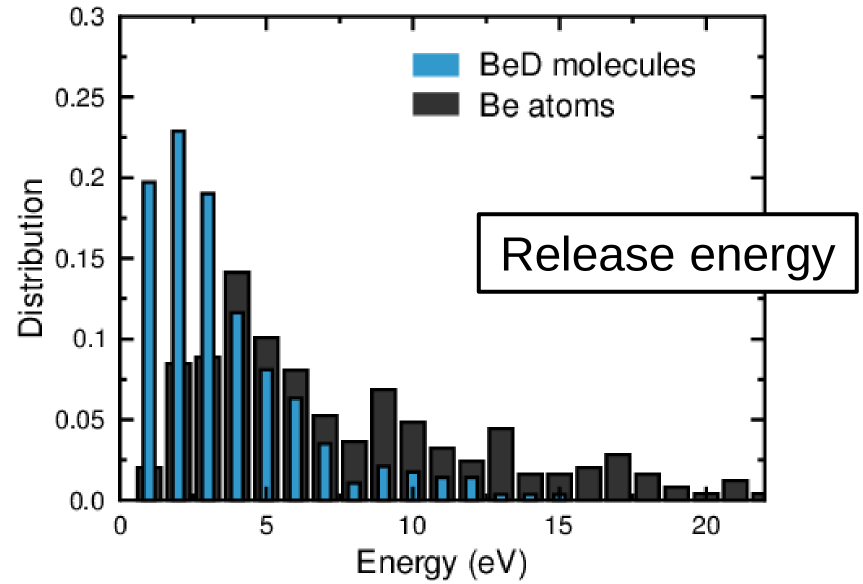
Swift chemical sputtering

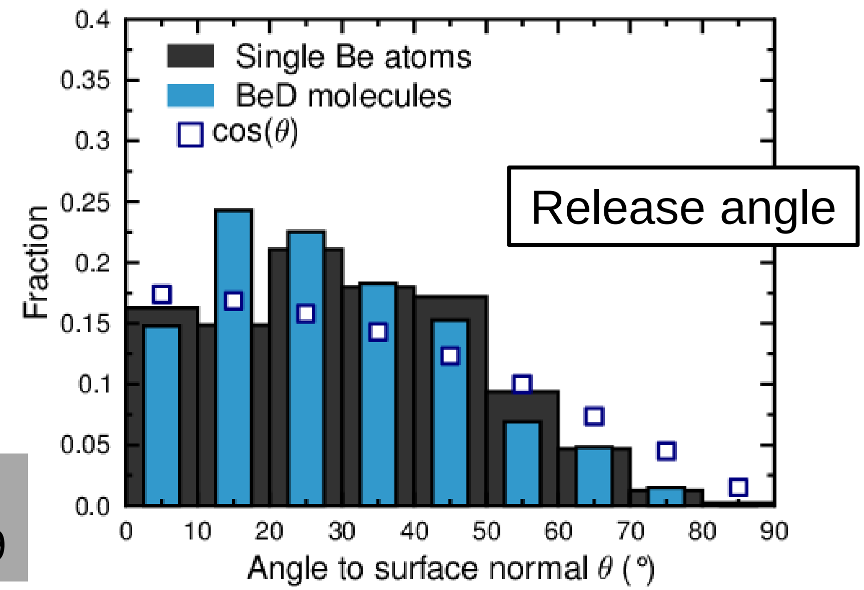
Snapshots of a single sputtering as an illustration for MD simulation



BeD implementation in ERO

- BeD yield:
  - 17% of total Be sputtering yield assumed in benchmark simulations for PISCES-B [*].
  - If surface T controlled, BeD fraction is ion energy dependent
- Sputtering and reflection:
  - MD: BeD sputters as single Be and has a low sticking
- Reactions in plasma:
  - BeD + e$^-$ collision rates calculated





[*] C. Björkas et al., J. Nucl. Mater. (2013), http://dx.doi.org/10.1016/j.jnucmat.2013.01.039

ERO input: BeD reactions in plasma

- BeD + e^- collision rates depend on T_e and vibrational state v
  - Assume v=1 and transitions Δv=0

Thanks for consultation to R.Janev

Important reactions

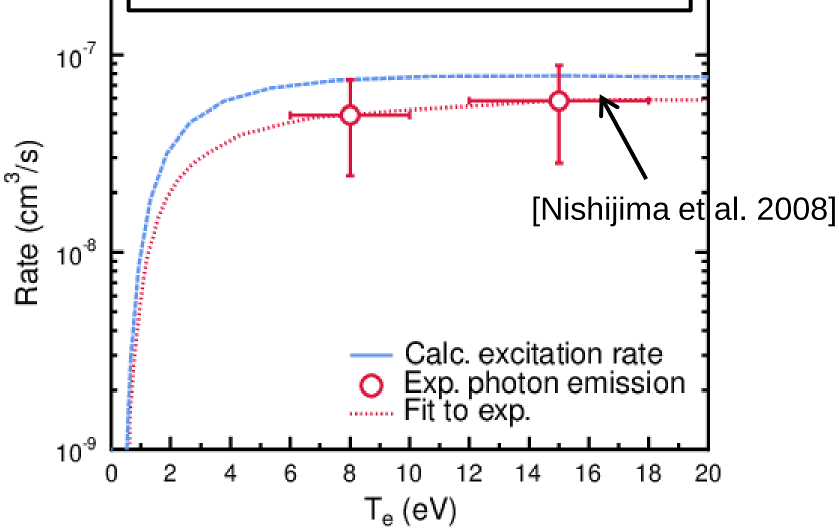
$$e + \mathrm{BeD} \rightarrow e + \mathrm{BeD}^+$$

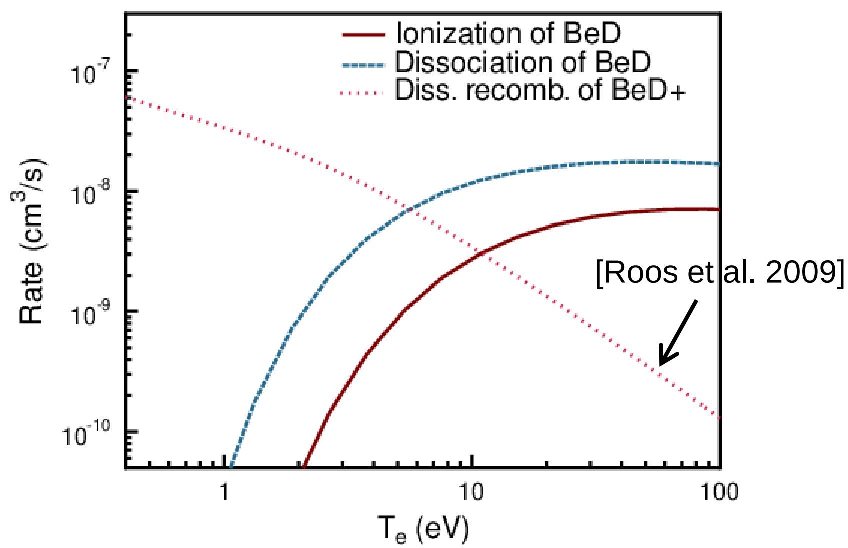
$$e + \mathrm{BeD} \rightarrow e + \mathrm{BeD}^*$$

$$e + \mathrm{BeD} \rightarrow$$
$$e + \mathrm{BeD}^*$$
$$\rightarrow e + \mathrm{Be}(3_P) + \mathrm{D}(1_S)$$

Metastable now!

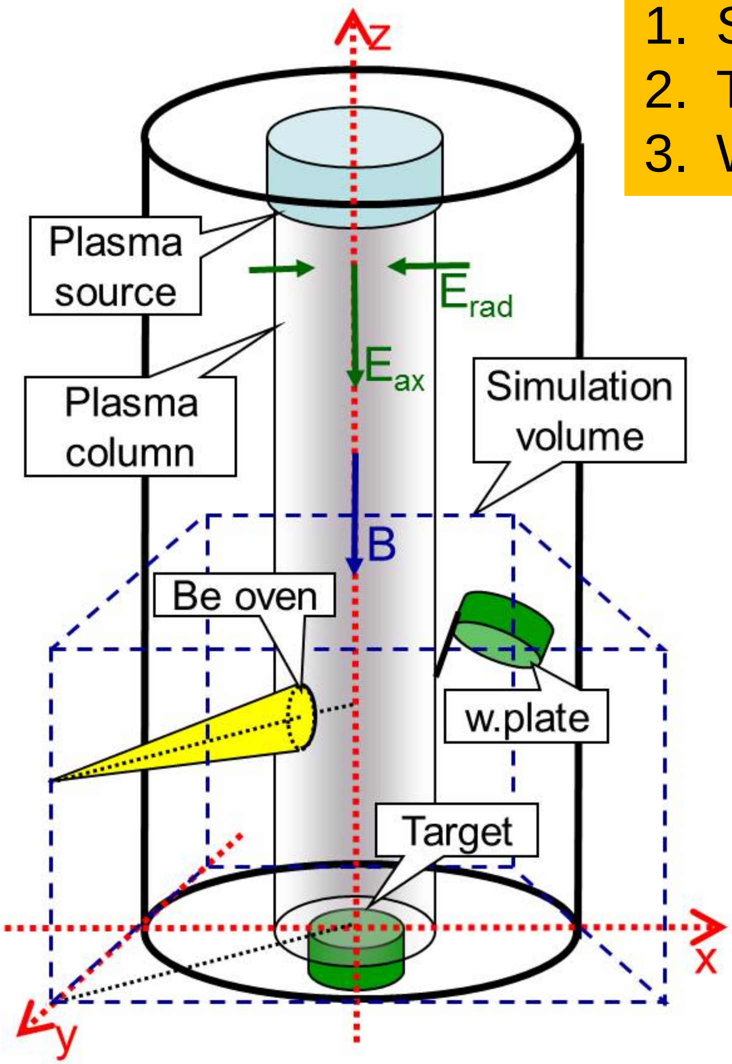
Photon emission coefficient





Linear devices

PISCES-B



Perfect for Be sputtering yields benchmark

1. Spectroscopy
2. Target weight loss
3. Witness plate

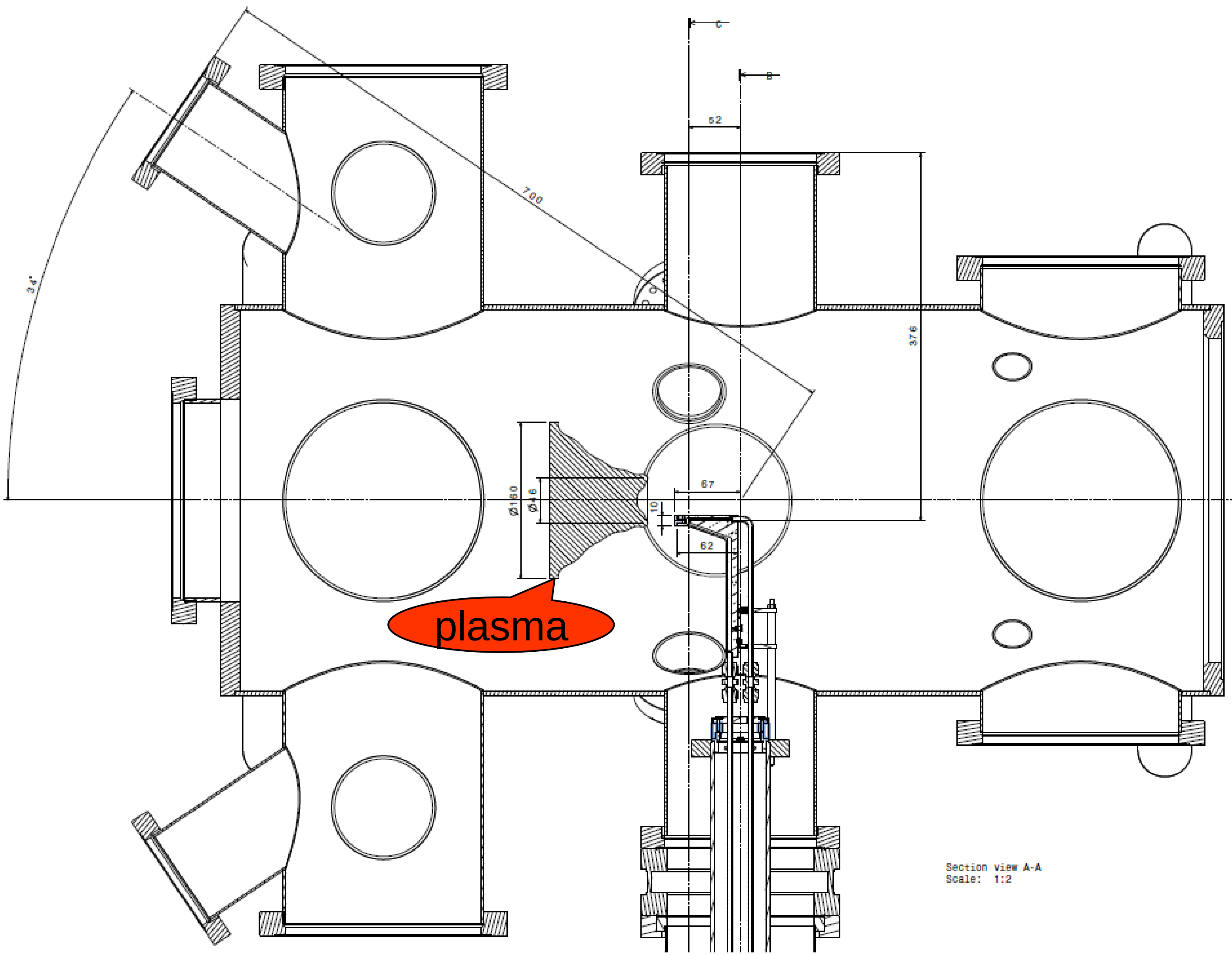
Also Pilot-PSI and **JULE-PSI**

Collaborations: **PISCES, FOM, MePhI**

Many physical effects introduced into the ERO code:

1) Elastic collisions
2) Molecular ions (D^{2+}, D^{3+})
3) ***Metastable states tracking***
4) Dissociative excitation for CH
5) ***Be-D molecules release and decay in plasma***

PSI-2 linear device (FZJ)



Many diagnostics, target analysis station

W spectroscopy, weight loss M.Laegner (FZJ)

Be proxy

ERO simulations – E.Marenkov (MePhi)

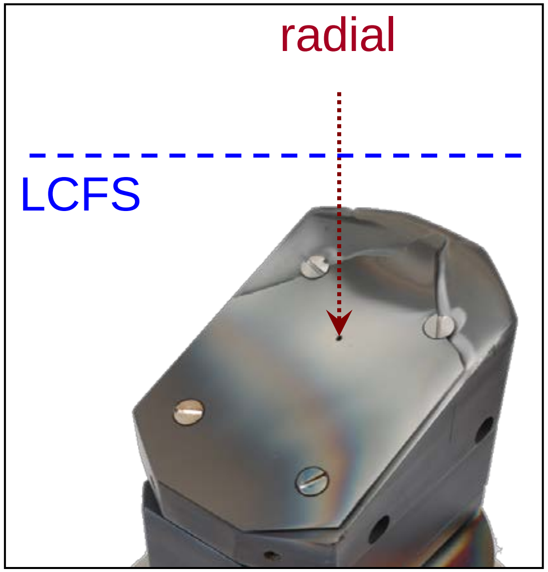
Drawing: A.Terra

W – most data is unavailable! . .

Physical issues: W influx, D/XB, erosion . . .

Sputtering experiments: badly known amount of particles (weight loss, markers)

WF_6 injection: Unknown dissociation, sticking rates and influence on emission



ERO: WF_6 injection, *roof limiter*

Dissociation data for WF_6 not available ⇒ in ERO:
inject W^0 atoms & *reduce ionisation rate for injected W^0 to match observed W^0 light*

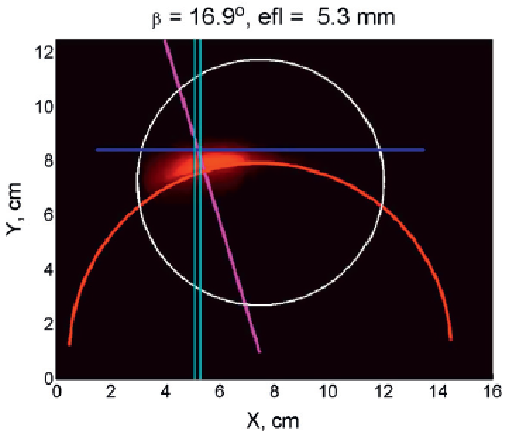
T_e(LCFS) = 30 eV
n_e(LCFS) = 5×10^{12} cm^{-3}
Ionisation rate for injected W^0 reduced by factor of 100!!!

ERO needs:

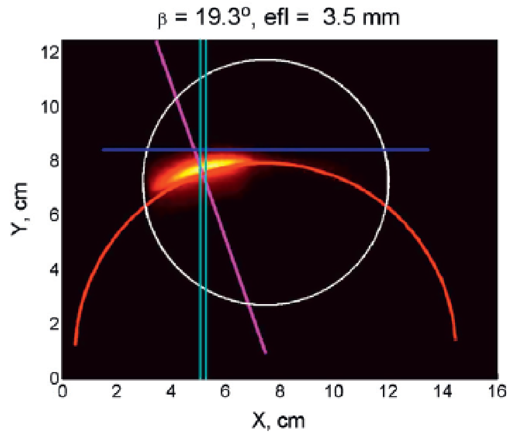
1) ionization of W^0, W^+, W^{2+}, effective PECs for "convenient" lines of WI, WII

2)a way to treat metastables and W-F molecules

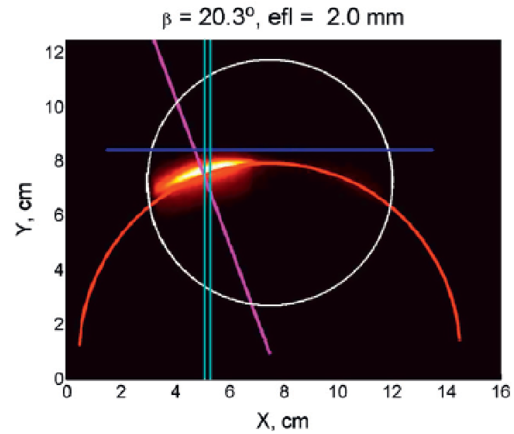
WI (400.9nm) light emission



Plasma cond. 1

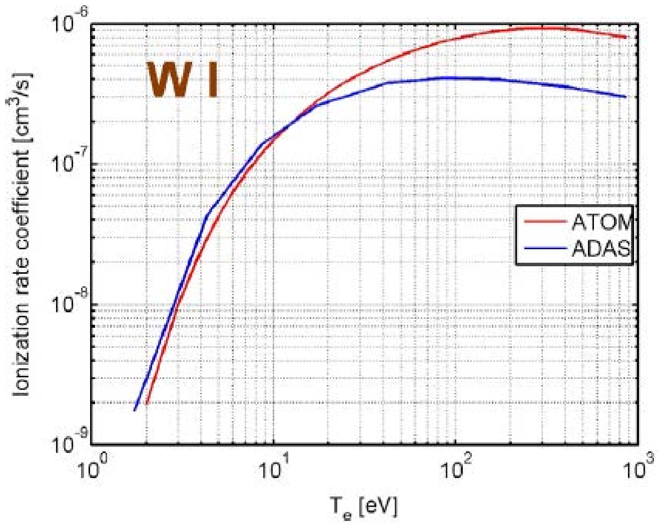


Plasma cond. 2



Plasma cond. 3

Fig. 1. W/C twin limiter after plasma exposure.



D. Kondratyev et al. / Journal of Nuclear Materials 438 (2013) S351–S355

ERO atomic/molecular data needs

1) **Atomic data** (**Be** (proxy: **Al**, Mg), **W**, **C**, D, He, Ar, . . .)

- ***Testing, reorganization, updating the database***
- ***Metastable tracking (sofar only for Be)***
- ***Tungsten, WF_6***

2) **Molecular data**

- Hydrocarbons – available (HYDKIN)
  - ***ERO simulations for TEXTOR, Pilot-PSI, . . .***
- Be-D molecules release, decay and spectroscopy
  - ***First ERO simulations for PISCES-B***
  - ***Ongoing – JET ILW***

ERO – bridge between fundamental data and multiple spectroscopic plasma experiments!

The End